

computational photochemistry

Aspects of research that address the study of photochemical events by means of computer simulations using specialized software tools and strategies in order to get an understanding of the process at a microscopic level. The aim is to uncover the mechanism of known photochemical processes, design new photochemical systems, and predict molecular properties that are experimentally inaccessible.

Source:

PAC, 2007, 79, 293 (*Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006)*) on page 316